RESEARCH ON SPECTROSCOPY, OPACITY, AND ATMOSPHERES

NASA Grant NAGW-4272

Annual Report No. 1

For the Period 1 January 1995 through 29 February 1996

Principal Investigator

Dr. Robert L. Kurucz

December 1996

Prepared for
National Aeronautics and Space Administration
Washington, D.C. 20546

Smithsonian Institution
Astrophysical Observatory
Cambridge, MA 02138

The Smithsonian Astrophysical Observatory
is a member of the
Harvard-Smithsonian Center for Astrophysics

The NASA Technical Officer for this Grant is Dr. Hashima Hasan, Code SR, Ultraviolet, Visible, and Gravitational Astrophysics, NASA Headquarters, Washington, D.C. 20546-0001.

RESEARCH ON SPECTROSCOPY, OPACITY, AND ATMOSPHERES

NASA Grant NAGW-4272

Annual Report, No. 1

For the period 1 January 1995 to 29 February 1996

The main acomplishment this year was the merging of all my atomic line data into one wavelength-sorted list that is simple to use. Here is the README file:

KURUCZ CD-ROM NO. 23 Atomic Line List

Robert L. Kurucz and Barbara Bell

Smithsonian Astrophysical Observatory

April 15, 1995

This line list is a replacement for the Kurucz-Peytremann line list. We have combined all the atomic files from CDROM 18 into 534910 line files GFALL.DAT and GFELEM.DAT. These are the data we actually use to compute spectra. They are not up to date. References are given in GFALL.REF or GFELEM.REF. There are no references after 1988. For light elements there are no references after 1979. We have the literature into the 1990's but have not had manpower or funding to update everything. Our current plan is to make a new semiempirical calculation for each species and at that time to include all the data from the literature.

One new development is the inclusion of hyperfine splitting for the iron group elements using hyperfine data from the literature through 1993. The data are very incomplete. We have not yet included data for isotopic splitting. We supply a program for splitting the line list for a species. It reads the hyperfine and isotopic splitting parameters for levels and computes the splittings whenever those levels appear. Lines with no splitting data are copied untouched. Because Sc, Mn, and Co are monoisotopic, only the hyperfine splittings are needed. Since 51V is much more abundant than 50V, the isotope shifts are small for 51V, and we approximate V with 51V. GFALLHYP.DAT has 754946 lines including hyperfine Sc I, V I, Mn I, and Co I,

DIRECTORY CDROM23	**filenames on CD are edited to 8 or fewer characters**
GFREADME.DAT	
CDROM23.BIGFILES	**GFALL.DAT, GFELEM.DAT, and GFALLHYP.DAT**
CDROM23.COMFILES	**.COM, .FOR, and .LOG files for sorting and splitting the big files into small files. GFALL.REF and GFELEM.REF. RGFALL.FOR, a sample program that can read these data files into SYNTHE (CDROM 18).**
CDROM23.GF10	**GF0010.10, etc. small files for nominal 10 nm intervals**

CDROM23.GF100	GF0100.100, etc.	medium files for nominal 100 nm intervals
CDROM23.GFALL	GF0100.ALL, etc.	file for each species
CDROM23.GFHY10	GFHY0010.10, etc.	small files including hyperfine lines for nominal 10 nm intervals
CDROM23.HYPERFIN	files for computing hyperfine splitting for individual isotopes	

THESE FILES ARE GUARANTEED TO CONTAIN ERRORS.

This research partially supported by NASA grants NAGW-1486, 2528, and 3299, and by a grant of Cray time at the San Diego Supercomputer Center.

To mount under VMS:
CD_MOUNT/MEDIA=CDROM/UNDEFINED=(STREAM_CR:132) <device> CDROM23 <logical name>

On some computers translate CR to LF:
In UNIX: tr '\015' '\012' < filename | more

I am producing a line list for the first five or ten ions of all atoms and for all relevant diatomic molecules. My current list of 58 million atomic and diatomic lines will be revised using new laboratory analyses that have become available since my line lists were prepared. Then I will concentrate on filling in the lighter and heavier elements that are poorly represented at present. I will continue to add hyperfine and isotopic spittings to the line list as I work on computing heavier and lighter elements. Additional diatomic molecules and bands will be added to fill in the ultraviolet. The line data will be distributed on CD-ROMs as they are produced.

I have started recomputing Fe I, Ni I, and V I using new analyses but I have not made much progress because of distractions from other projects such as determining the primordial lithium abundance and getting a new opacity sampling model atmosphere program to work.

Here is my bibliography for the last year:

1994 Solar abundance model atmospheres for 0,1,2,4,8 km/s. Kurucz CD-ROM No. 19.

1994 Atomic Data for Ca, Sc, Ti, V, and Cr. Kurucz CD-ROM No. 20.

1994 Atomic Data for Mn and Co. Kurucz CD-ROM No. 21.

1994 Atomic Data for Fe and Ni. Kurucz CD-ROM No. 22.

1994 Synthetic DDO colours. (C. Morosso, M. Franchini, M.L. Malagnini, R.L. Kurucz, and R. Buser) Astron. Astrophys. vol. 295, pp. 471-478.

1994 An upper limit for the deuterium abundance in the halo star HD 140283. (D.A. Lubowich, J.M. Pasachoff, R.P. Galloway, R.L. Kurucz, and V.V. Smith) Bull. Amer. Astron. Soc., vol. 26, 1479.

1995 Synthetic template spectra. Presented at Joint Discussion 12, Accuracy of the HR Diagram and Related Parameters, at the 22nd General Assembly of the International Astronomical Union, the Hague, 14 - 27 August 1994. Highlights of Astronomy (ed. I. Appenzeller), vol. 10, 407-410.

1995 The Kurucz atomic and molecular database. Presented at Joint Discussion 16, Astrophysical Applications of Powerful New Atomic Databases, at the 22nd General Assembly of the International Astronomical Union, the Hague, 14 - 27 August 1994. Proceedings to be published.

1995 The solar spectrum: atlases and line identifications. Presented at the Workshop on Laboratory and Astronomical High Resolution Spectra, 29 August - 2 September 1994, Brussels. In Laboratory and Astronomical High Resolution Spectra, Astron. Soc. of the Pacific Conf. Series 81, (eds. A.J. Sauval, R. Blomme, and N. Grevesse) San Francisco: Astron. Soc. of the Pacific, pp. 17-31.

1995 An atomic and molecular data bank for stellar spectroscopy. Presented at the Workshop on Laboratory and Astronomical High Resolution Spectra, 29 August - 2 September 1994, Brussels. In Laboratory and Astronomical High Resolution Spectra, Astron. Soc. of the Pacific Conf. Series 81, (eds. A.J. Sauval, R. Blomme, and N. Grevesse) San Francisco: Astron. Soc. of the Pacific, pp. 583-588.

1995 The spectrum of Sirius from 307 to 1040 nm. (I. Furenlid, R.L. Kurucz, and T. Westin) Presented at the Workshop on Laboratory and Astronomical High Resolution Spectra, 29 August - 2 September 1994, Brussels. In Laboratory and Astronomical High Resolution Spectra, Astron. Soc. of the Pacific Conf. Series 81, (eds. A.J. Sauval, R. Blomme, and N. Grevesse) San Francisco: Astron. Soc. of the Pacific, pp. 615-616.

1995 Atomic Line Data (R.L. Kurucz and B. Bell) Kurucz CD-ROM No. 23.

1995 Rapid calculation of line opacity. To appear in Computational Astrophysics, Volume 2, Stellar Physics (ed. R. Kudritzki, D. Mihalas, K. Nomoto, and F.-K. Thielemann) Springer-Verlag, Berlin.

1995 The primordial lithium abundance. Astrophys. Journ. Oct 10 issue.

I will produce the following CDs as an ongoing program:

ATLAS12 opacity sampling model atmosphere program that allows arbitrary abundances that can vary with depth.

Model Atmosphere Grids: [-0.5a],[+0.0a],[+0.5a] 2 km/s for bulge stars, where "a" stands for alpha-process elements enhanced by +0.4 in the log
Model Atmosphere Grids: [-1.0a],[-1.5a],[-2.0a] 2 km/s.
Model Atmosphere Grids: [-2.5a],[-3.0a],[-3.5a] 2 km/s.
Model Atmosphere Grids: [-4.0a],[-4.5a],[-5.0a] 2 km/s.
Model Atmosphere Grids: [-0.5] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [-1.0] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [-1.5] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [-2.0] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [+0.5] for 0,1,2,4,8 km/s Vturb.

Model Atmosphere Grids: [+0.0a] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [-0.5a] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [-1.0a] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [-1.5a] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [-2.0a] for 0,1,2,4,8 km/s Vturb.
Model Atmosphere Grids: [+0.5a] for 0,1,2,4,8 km/s Vturb.

I can now work on stars considering flux and spectrum data simultaneously in the ultraviolet, visible, and infrared. I can compute a spectrum including all 58 million lines (or just the ones with good wavelengths) at full resolution from the ultraviolet to the infrared for any model.

I am working with Fiorella Castelli at Trieste on understanding the ultraviolet spectra of Vega and Sirius, with Glen Wahlgren of Goddard on an atlas of the GHRS spectrum of Sirius, and with Alfred Vidal-Madjar, IAP Paris, on the Fe II and Cr II emission lines seen around the core of his GHRS Lyman alpha spectrum of Sirius.